Supporting Information

Efficient and Robust Host-Guest Antenna Composite for Light Harvesting

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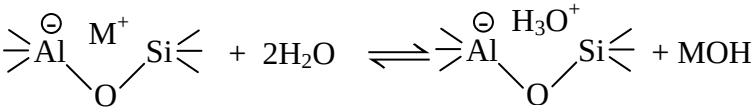
Discussion of the effects of metal cations on the proton activity in the channels of ZL

Hydrolysis leads to the formation of Brønsted sites as explained in Eq. SI1, which shows a simplified view of a zeolite represented by two TO_4 units and a monovalent cation M^+ as charge compensating counter ion.[42] This reaction corresponds to reaction Eq. (4a). It explains the common experimental observation that metal cation exchanged ZL in distilled water lead to basic solutions whereas at the same time the proton concentration and, therefore, the acidity inside the cavity increases.



(SI1)

The reaction can formally be represented as follows.

$$ZLO^-M^+ + 2H_2O \rightleftharpoons ZLO^-H_3O^+ + M^+OH^- \quad \text{(SI2)}$$

With the equilibrium constant K

$$K = \frac{a(ZLO^-H_3O^+)a(M^+OH^-)}{a(ZLO^-M^+)a(H_2O)^2} \quad \text{(SI3)}$$

Using the abbreviation C_0 for the total concentration of M^+, the fact that $a(ZLO^-H_3O^+) = a(M^+OH^-)$ holds and abbreviating this for simplicity as $a(H_3O^+)$ we find:

$$a(H_3O^+) = \frac{1}{2}Ka(H_2O)^2\left[\sqrt{1+4\frac{C_0}{Ka(H_2O)^2}}-1\right] \quad \text{(SI4)}$$

Experimentally a pH of about 3.4 is found inside of the channels for hydrated potassium exchanged ZL L and 3.7 if potassium is exchanged by Cs^+.[32,33] Reading equation (SI4) we observe that the proton activity decreases with decreasing potassium concentration and it also decreases with decreasing amount of water present in the cavities. Both factors are favorably influenced when substituting part or all exchangeable potassium cations by IMZ^+ because IMZ^+ not only decreases the amount of potassium present, it also reduces the space available for water molecules, and it acts by itself as a weak base.